



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:14 AM UTC

PDB ID : 1B40 / pdb_00001b40
Title : OLIGO-PEPTIDE BINDING PROTEIN (OPPA) COMPLEXED WITH KFK
Authors : Tame, J.R.H.; Wilkinson, A.J.
Deposited on : 1998-11-23
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

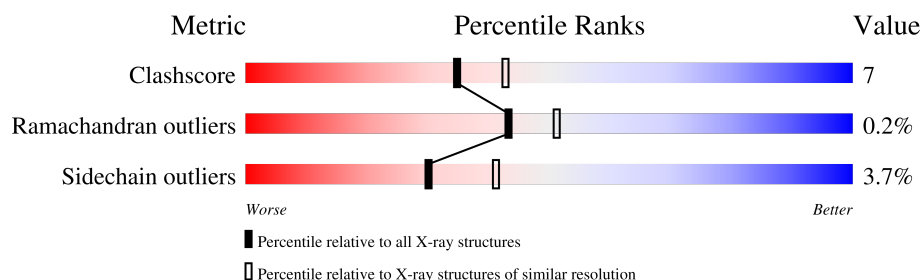
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

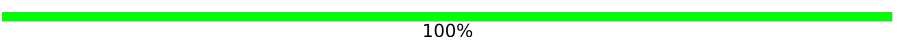
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	517	 72% 23% . .
2	B	3	 100%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4364 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

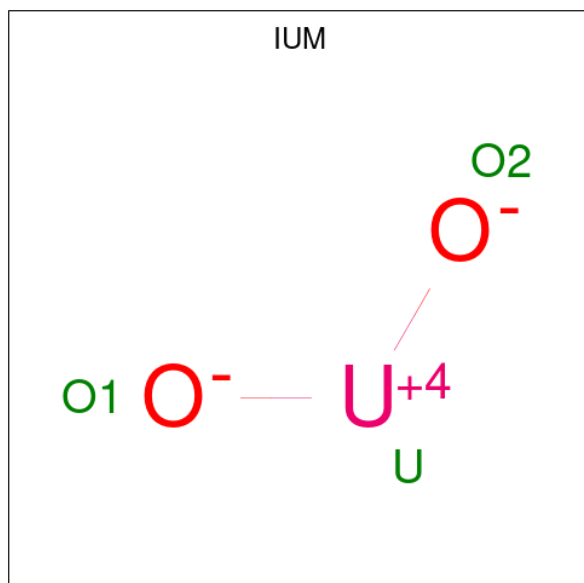
- Molecule 1 is a protein called PROTEIN (OLIGO-PEPTIDE BINDING PROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	0	0
			4164	2666	700	793	5			

- Molecule 2 is a protein called PROTEIN (LYS-PHE-LYS).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			29	21	5	3			

- Molecule 3 is URANYL (VI) ION (CCD ID: IUM) (formula: O₂U).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	U	0	0
			1	1		
3	A	1	Total	U	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	U 1	0	0
3	A	1	Total 1	U 1	0	0
3	A	1	Total 1	U 1	0	0
3	A	1	Total 1	U 1	0	0
3	A	1	Total 1	U 1	0	0
3	A	1	Total 1	U 1	0	0

- Molecule 4 is water.

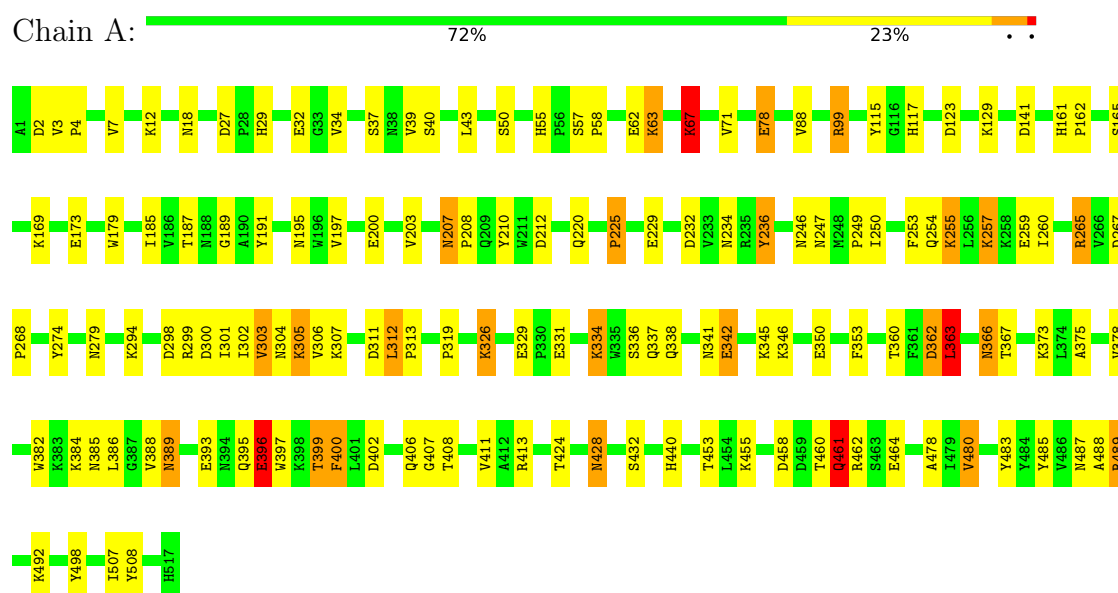
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	163	Total 163	O 163	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: PROTEIN (OLIGO-PEPTIDE BINDING PROTEIN)



• Molecule 2: PROTEIN (LYS-PHE-LYS)



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.69Å 75.16Å 69.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20	Depositor
% Data completeness (in resolution range)	98.4 (15.00-2.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.199 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4364	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: IUM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.77	0/4275	1.81	78/5830 (1.3%)
2	B	0.77	0/29	1.09	0/35
All	All	0.77	0/4304	1.80	78/5865 (1.3%)

There are no bond length outliers.

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	GLU	CB-CG-CD	14.73	137.65	112.60
1	A	353	PHE	CA-CB-CG	-9.08	104.72	113.80
1	A	366	ASN	OD1-CG-ND2	8.82	131.42	122.60
1	A	247	ASN	CA-CB-CG	8.16	120.77	112.60
1	A	34	VAL	CA-C-O	7.93	124.00	118.69
1	A	246	ASN	CA-C-N	7.63	133.69	122.39
1	A	246	ASN	C-N-CA	7.63	133.69	122.39
1	A	234	ASN	CA-C-O	-7.50	112.61	120.55
1	A	362	ASP	CA-C-O	7.30	129.90	121.28
1	A	407	GLY	N-CA-C	-7.30	105.16	115.30
1	A	341	ASN	CA-CB-CG	7.17	119.77	112.60
1	A	389	ASN	CA-CB-CG	-7.01	105.59	112.60
1	A	234	ASN	N-CA-CB	6.78	120.08	110.12
1	A	274	TYR	CA-C-O	-6.75	114.04	121.33
1	A	408	THR	N-CA-CB	6.75	118.95	110.45
1	A	485	TYR	CA-CB-CG	6.67	125.90	113.90
1	A	489	ARG	CD-NE-CZ	6.64	133.70	124.40
1	A	400	PHE	CA-C-O	-6.61	113.88	120.82
1	A	117	HIS	CA-CB-CG	-6.58	107.22	113.80
1	A	386	LEU	N-CA-CB	-6.55	102.33	110.98
1	A	39	VAL	CA-C-O	-6.53	113.93	120.85
1	A	399	THR	CA-C-O	6.42	127.23	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	TYR	CA-C-N	6.35	132.53	122.62
1	A	191	TYR	C-N-CA	6.35	132.53	122.62
1	A	299	ARG	CD-NE-CZ	6.26	133.16	124.40
1	A	375	ALA	CA-C-O	6.16	127.08	120.55
1	A	50	SER	CA-C-O	-6.12	114.08	121.05
1	A	185	ILE	CA-C-O	6.08	127.86	121.59
1	A	274	TYR	O-C-N	6.08	130.18	123.25
1	A	432	SER	CA-CB-OG	-5.90	99.30	111.10
1	A	99	ARG	NE-CZ-NH1	-5.88	115.62	121.50
1	A	303	VAL	N-CA-C	5.83	116.47	110.82
1	A	232	ASP	CA-CB-CG	5.70	118.30	112.60
1	A	141	ASP	CA-CB-CG	5.66	118.26	112.60
1	A	88	VAL	CA-C-O	-5.52	114.47	120.71
1	A	480	VAL	N-CA-CB	5.51	118.92	111.21
1	A	411	VAL	CA-C-O	-5.51	114.50	120.67
1	A	385	ASN	CA-C-N	-5.44	113.65	121.98
1	A	385	ASN	C-N-CA	-5.44	113.65	121.98
1	A	234	ASN	O-C-N	5.39	127.84	122.12
1	A	384	LYS	CA-CB-CG	5.39	124.87	114.10
1	A	18	ASN	N-CA-CB	5.36	118.44	110.29
1	A	32	GLU	CA-C-N	-5.35	116.92	122.69
1	A	32	GLU	C-N-CA	-5.35	116.92	122.69
1	A	179	TRP	CA-CB-CG	5.33	123.73	113.60
1	A	2	ASP	CA-C-O	-5.30	114.59	121.11
1	A	319	PRO	CA-C-N	5.29	124.90	119.56
1	A	319	PRO	C-N-CA	5.29	124.90	119.56
1	A	257	LYS	CA-CB-CG	5.26	124.62	114.10
1	A	220	GLN	CA-C-N	-5.25	115.65	122.94
1	A	220	GLN	C-N-CA	-5.25	115.65	122.94
1	A	67	LYS	CB-CA-C	5.24	119.17	110.74
1	A	489	ARG	NE-CZ-NH1	5.22	126.72	121.50
1	A	55	HIS	CB-CA-C	-5.21	101.60	109.26
1	A	363	LEU	CB-CA-C	5.21	118.48	110.62
1	A	37	SER	CA-C-O	-5.20	114.00	119.97
1	A	336	SER	N-CA-C	-5.19	103.54	110.55
1	A	189	GLY	O-C-N	-5.17	117.96	122.88
1	A	207	ASN	CA-C-O	5.16	123.69	119.36
1	A	78	GLU	N-CA-C	5.14	117.78	111.82
1	A	225	PRO	N-CA-CB	-5.13	97.86	103.25
1	A	27	ASP	CA-C-N	5.12	125.41	119.47
1	A	27	ASP	C-N-CA	5.12	125.41	119.47
1	A	260	ILE	CA-C-N	5.11	124.56	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	ILE	C-N-CA	5.11	124.56	119.24
1	A	428	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	A	411	VAL	O-C-N	5.11	128.57	123.10
1	A	326	LYS	N-CA-CB	5.11	119.86	111.58
1	A	389	ASN	OD1-CG-ND2	5.09	127.69	122.60
1	A	508	TYR	CA-C-O	-5.09	114.86	120.36
1	A	487	ASN	CA-CB-CG	-5.09	107.51	112.60
1	A	440	HIS	CA-CB-CG	-5.08	108.72	113.80
1	A	265	ARG	CD-NE-CZ	5.08	131.51	124.40
1	A	461	GLN	CA-CB-CG	-5.08	103.94	114.10
1	A	342	GLU	CB-CG-CD	5.06	121.20	112.60
1	A	236	TYR	N-CA-C	-5.04	105.43	111.03
1	A	165	SER	CA-C-O	5.04	125.13	120.60
1	A	40	SER	N-CA-C	5.00	116.73	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4164	0	4076	62	1
2	B	29	0	37	0	0
3	A	8	0	0	0	1
4	A	163	0	0	2	0
All	All	4364	0	4113	62	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (62) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LYS:HA	1:A:480:VAL:HG13	1.69	0.73
1:A:169:LYS:HE2	1:A:173:GLU:OE2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:THR:O	1:A:464:GLU:HG3	1.93	0.69
1:A:326:LYS:HD2	4:A:678:HOH:O	1.98	0.63
1:A:307:LYS:HE3	1:A:483:TYR:OH	1.99	0.62
1:A:257:LYS:HG2	4:A:683:HOH:O	2.03	0.58
1:A:458:ASP:HB3	1:A:461:GLN:HB2	1.87	0.56
1:A:402:ASP:O	1:A:406:GLN:HG3	2.07	0.54
1:A:453:THR:HB	1:A:462:ARG:HG3	1.88	0.54
1:A:195:ASN:HB2	1:A:203:VAL:HB	1.90	0.54
1:A:255:LYS:HD2	1:A:259:GLU:OE2	2.08	0.54
1:A:396:GLU:HG2	1:A:397:TRP:N	2.21	0.53
1:A:62:GLU:HG3	1:A:63:LYS:HD2	1.90	0.53
1:A:115:TYR:CE1	1:A:428:ASN:HB3	2.44	0.53
1:A:301:ILE:HA	1:A:305:LYS:HG3	1.90	0.52
1:A:301:ILE:HA	1:A:305:LYS:CG	2.40	0.52
1:A:250:ILE:HB	1:A:373:LYS:HD3	1.92	0.51
1:A:300:ASP:OD1	1:A:304:ASN:ND2	2.40	0.51
1:A:345:LYS:HB2	1:A:345:LYS:NZ	2.26	0.51
1:A:43:LEU:O	1:A:187:THR:HB	2.11	0.50
1:A:382:TRP:HB3	1:A:388:VAL:CG2	2.41	0.50
1:A:345:LYS:HB2	1:A:345:LYS:HZ2	1.76	0.49
1:A:265:ARG:O	1:A:488:ALA:HA	2.12	0.49
1:A:123:ASP:HB3	1:A:129:LYS:HG3	1.95	0.48
1:A:395:GLN:NE2	1:A:399:THR:HG22	2.29	0.48
1:A:489:ARG:NH1	1:A:498:TYR:OH	2.40	0.48
1:A:424:THR:HB	1:A:428:ASN:ND2	2.29	0.47
1:A:197:VAL:HB	1:A:200:GLU:HB3	1.96	0.47
1:A:366:ASN:O	1:A:367:THR:C	2.55	0.47
1:A:346:LYS:O	1:A:350:GLU:HG3	2.15	0.47
1:A:210:TYR:CE2	1:A:212:ASP:HB3	2.51	0.46
1:A:236:TYR:CZ	1:A:492:LYS:HE3	2.50	0.46
1:A:115:TYR:CD1	1:A:428:ASN:HB3	2.51	0.46
1:A:279:ASN:HD21	1:A:478:ALA:HA	1.80	0.46
1:A:123:ASP:CB	1:A:129:LYS:HG3	2.46	0.46
1:A:402:ASP:OD2	1:A:406:GLN:NE2	2.49	0.46
1:A:302:ILE:HD11	1:A:378:VAL:HG22	1.97	0.45
1:A:342:GLU:CD	1:A:345:LYS:HZ1	2.23	0.45
1:A:29:HIS:ND1	1:A:99:ARG:NH1	2.65	0.45
1:A:329:GLU:OE2	1:A:334:LYS:HE3	2.17	0.45
1:A:123:ASP:OD2	1:A:129:LYS:NZ	2.46	0.44
1:A:298:ASP:OD2	1:A:337:GLN:HG2	2.18	0.44
1:A:302:ILE:CD1	1:A:378:VAL:HG22	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ASP:HB3	1:A:268:PRO:CD	2.48	0.44
1:A:161:HIS:CD2	1:A:162:PRO:HD2	2.53	0.43
1:A:312:LEU:HA	1:A:313:PRO:HD3	1.92	0.43
1:A:3:VAL:HA	1:A:4:PRO:HD3	1.87	0.43
1:A:207:ASN:HA	1:A:208:PRO:HD2	1.90	0.43
1:A:229:GLU:HB3	1:A:249:PRO:HD3	2.01	0.43
1:A:303:VAL:HG13	1:A:311:ASP:HB2	2.01	0.42
1:A:363:LEU:C	1:A:363:LEU:HD12	2.45	0.42
1:A:57:SER:HB3	1:A:58:PRO:HD2	2.02	0.42
1:A:267:ASP:HB3	1:A:268:PRO:HD2	2.01	0.41
1:A:312:LEU:O	1:A:313:PRO:C	2.62	0.41
1:A:67:LYS:HE2	1:A:71:VAL:HG21	2.03	0.41
1:A:362:ASP:OD1	1:A:362:ASP:N	2.53	0.41
1:A:253:PHE:O	1:A:254:GLN:C	2.64	0.41
1:A:331:GLU:OE2	1:A:334:LYS:NZ	2.44	0.41
1:A:360:THR:HA	1:A:389:ASN:O	2.21	0.41
1:A:366:ASN:HB3	1:A:400:PHE:CD2	2.56	0.41
1:A:236:TYR:CE1	1:A:492:LYS:HE3	2.56	0.40
1:A:362:ASP:OD2	1:A:393:GLU:OE2	2.40	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:GLU:OE2	3:A:525:IUM:U[1_556]	1.94	0.26

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	515/517 (100%)	496 (96%)	18 (4%)	1 (0%)	43 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1/3 (33%)	1 (100%)	0	0	100	100
All	All	516/520 (99%)	497 (96%)	18 (4%)	1 (0%)	43	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	455/455 (100%)	438 (96%)	17 (4%)	30	41
2	B	3/3 (100%)	3 (100%)	0	100	100
All	All	458/458 (100%)	441 (96%)	17 (4%)	30	41

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	12	LYS
1	A	63	LYS
1	A	67	LYS
1	A	78	GLU
1	A	255	LYS
1	A	305	LYS
1	A	306	VAL
1	A	312	LEU
1	A	334	LYS
1	A	338	GLN
1	A	363	LEU
1	A	396	GLU
1	A	413	ARG
1	A	455	LYS

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Mol	Chain	Res	Type
1	A	461	GLN
1	A	507	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	117	HIS
1	A	199	ASN
1	A	279	ASN
1	A	308	ASN
1	A	395	GLN
1	A	428	ASN
1	A	440	HIS
1	A	461	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are modelled with single atom - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.